Diagrammatic Expansion for Positive Spectral Functions in the Steady-State Limit

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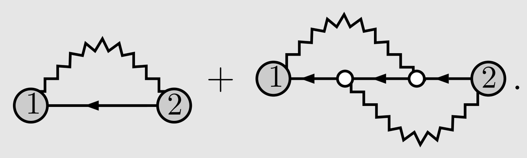
Abstract

Recently, a method was presented [1] for constructing self-energies within many-body perturbation theory that are guaranteed to produce a positive spectral function for equilibrium systems, by representing the self-energy as a product of half-diagrams on the forward and backward branches of the Keldysh contour. We derive an alternative half-diagram representation that is based on products of retarded diagrams. Our approach extends the method to systems out of equilibrium. When a steady-state limit exists, we show that our approach yields a positive definite spectral function in the frequency domain.

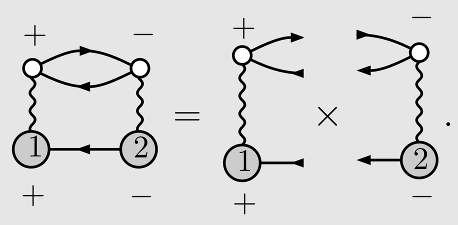
1. The Problem

- Some approximations for the self-energy can lead to negative valued spectral functions.
- This prevents the probability interpretation of the spectral function, and can lead to instability in self-consistent calculations.
- This issue arises for example for:

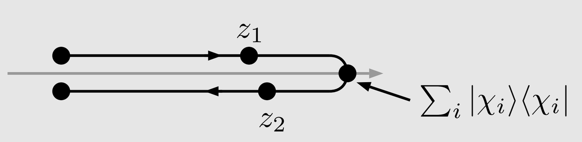
$\Sigma_{xc}(z_1, z_2) =$  (1)

2. Self-Energy in Terms of Half-Diagrams

- In Ref. [1] it was shown that in zero temperature the spectral function will be positive semi-definite (PSD) if the self-energy can be represented as a sum of squares of half-diagrams.
- For example

 (2)

- This splitting is obtained by placing a complete basis set at the end-point of the contour at $t = \infty$:



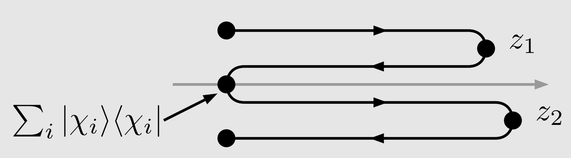
(3)

- The half-diagrams are then (anti)-time ordered.
- This requires the assumption that the initial state $|\Phi_0\rangle$ is connected to the state obtained in the distant future:

$$\mathcal{U}(\infty, -\infty)|\Phi_0\rangle = e^{i\alpha}|\Phi_0\rangle. \tag{4}$$

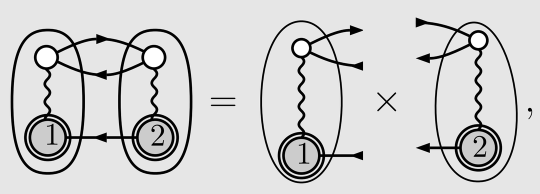
3. Generalization to Steady-State

- In Ref. [2] we show that the same proof can be performed without the assumption in Eq.(4), by placing the basis set at $t = -\infty$:



(5)

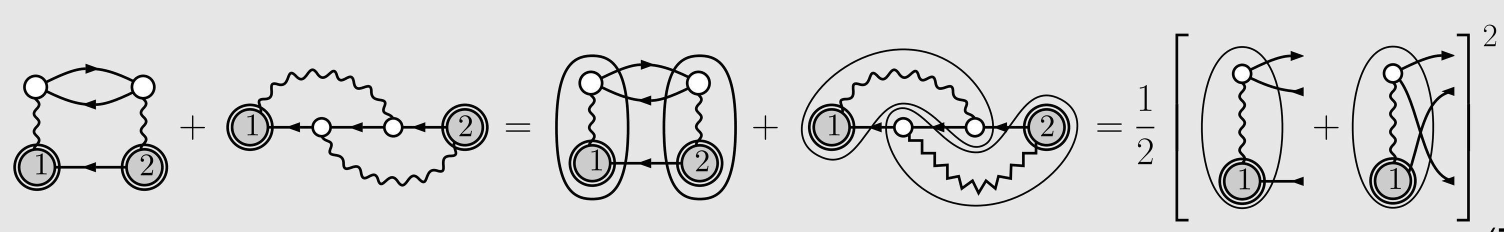
- The PSD nature of the spectral function can now be shown in the steady-state limit.
- In this case the half-diagrams are no longer time-ordered, but retarded. For example

 (6)

where the circling of vertices denotes a retarded piece, the other vertices being retarded with respect to the vertex marked with a double circle.
- In a general half-diagram all internal vertices are retarded with respect to vertex 1 (or 2). This requires defining a general retarded diagram [2].

4. Example: Second Born Approximation

The $2B$ approximation is PSD, since

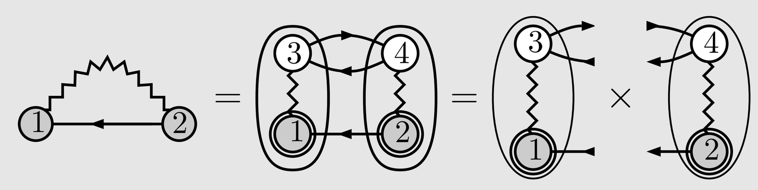
 (7)

5. Example: gW Approximation

The gW approximation with the RPA polarization funtion $P(1,2) = g(1,2)g(2,1)$ is PSD, since using

$$W^{\lessgtr}(1,2) = \int d3d4 W^R(1,3)P^{\lessgtr}(3,4)W^A(4,2) \tag{8}$$

we can write the xc-self-energy as

$\Sigma^{\lessgtr}_{xc,gW} =$  (9)

6. Generalized Retarded Compositions

- In order to define general retarded compositions, we will first define general contour ordered components
- A contour function that is representable as a diagram can be replaced by a real-time function whenever the order along the contour γ is fixed. For example

$$\bar{\Sigma}_{xc}(z_a, z_b, z_c, z_d) = \bar{\Sigma}^{1234}_{xc}(t_a, t_b, t_c, t_d) \text{ when } z_a > z_b > z_c > z_d. \tag{10}$$

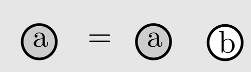
- For a two-point function these components are equal to the greater and lesser components:

$$G^{12}(z_a, z_b) = G^{>}(z_a, z_b), \qquad G^{21}(z_a, z_b) = G^{<}(z_a, z_b) \tag{11}$$

This set of functions for each permutation of the arguments encodes all the information in the original contour function.

6.1 One Vertex

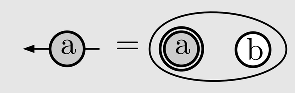
Take for example a half-diagram with a single internal vertex (with diagrammatic representation on the right):

$$D(z_a) = \int_\gamma dz_b D(z_a, z_b)$$  (12)

If one defines a retarded composition

$$D^R(t_a, t_b) = \theta(t_a - t_b)\big(D^{>}(t_a, t_b) - D^{<}(t_a, t_b)\big) = \theta_{ab}O^{[1,2]}(t_a, t_b), \tag{13}$$

it follows that

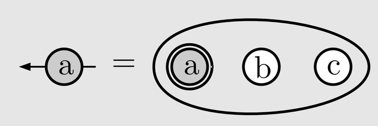
$$D^1(t_a) = \int_{t_0}^{\infty} dt_b D^R(t_a, t_b)$$  (14)

6.2 Two Vertices

A half-diagram with two internal vertices

$$D(z_a) = \int_\gamma dz_b dz_c D(z_a, z_b, z_c)$$  (15)

motivates the definition of a retarded composition for which

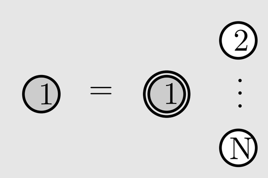
$$D^1(t_a) = \int_{t_0}^{\infty} dt_b dt_c D^{R(1,23)}(t_a, t_b, t_c)$$  (16)

This is achieved for example by

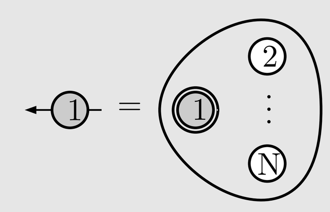
$$D^{R(1,23)} = \theta_{abc}D^{[[1,2],3]} + \theta_{acb}O^{[[1,3],2]}. \tag{17}$$

6.3 N Vertices

For a general half-diagram with N internal vertices

$$D(z_{n_1}) = \int_\gamma dz_{n_2} dz_{n_N} D(z_{n_1}, \dots, z_{n_N})$$  (18)

one then has

$$D^1(t_{n_1}) = \int_{t_0}^{\infty} dt_{n_2} \cdots dt_{n_N} D^{R(1,2\cdots n)}(t_{n_1}, \dots, t_{n_N})$$  (19)

with the retarded composition

$$D^{R(1,2\cdots n)} = \sum_{P \in S_{n-1}} \theta_{1P(2)\cdots P(n)} D^{[1,P(2),\dots,P(n)]} \tag{20}$$

References

[1] G. Stefanucci, Y. Pavlyukh, A.M. Uimonen, and R. van Leeuwen, Phys. Rev. B 90, 115134 (2014).

[2] M. J. Hyrkäs, D. Karlsson, and R. van Leeuwen *Contour calculus for many-particle functions*, to be published